Investigation of Portable Event-Based Monte Carlo Transport

COE Phoenix, AZ

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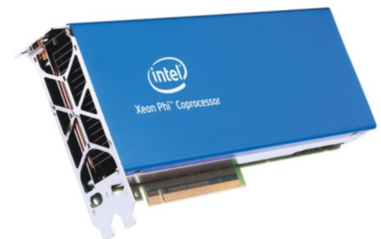
Current Landscape of Architectures

- GPU (NVIDIA)
  - Sub-architectures :
    - Fermi, Kepler, Maxwell
  - Multiple Memory Types:
    - Global, shared, constant, texture
  - Memory Amount:
    - Up to 12 GB
  - 1000s of threads
    - Grids, blocks, and warps

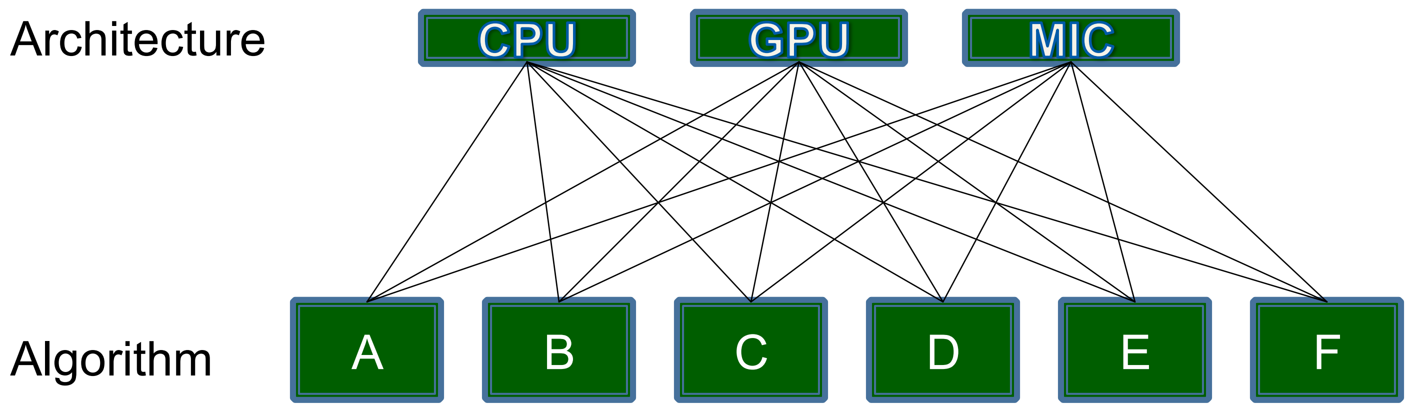


- CPU/MIC
  - Multiple ISAs:
    - Vector Unit Widths:
      - » 2,4,8 / 16
  - Single Memory Type
    - Shared/private caches
  - Larger Memory Size (CPU)
  - Up to 20/60 threads
    - No explicit organization

*Slide courtesy of Matthew Larsen
University of Oregon, CDUX research group

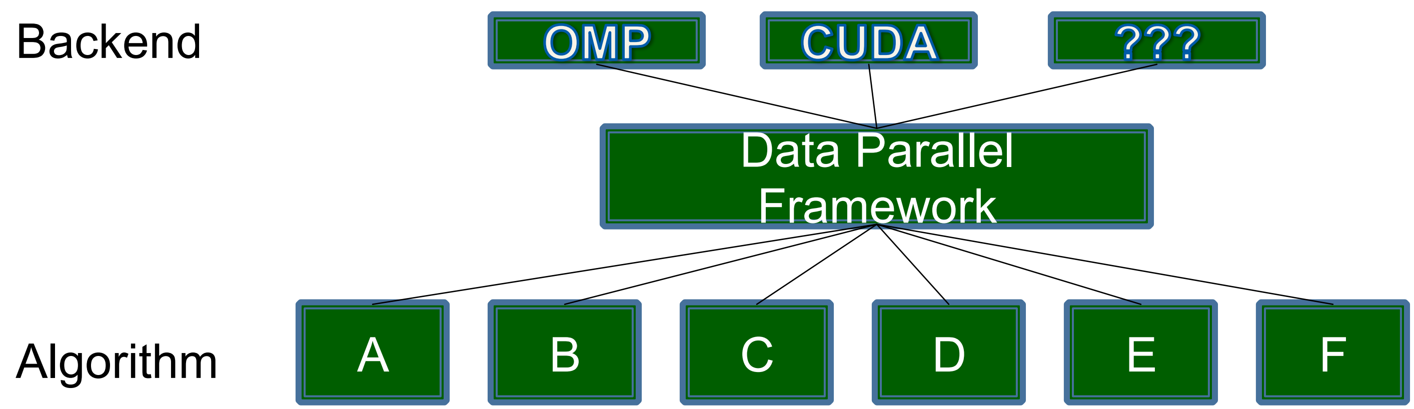
The Problem

- Forces developers to either:
  - Pick a target architecture
  - Add additional implementations of the same algorithm:



Data-Parallel Primitives Libraries

- Backend – Implement fast parallel primitive operators for each new architecture
- Frontend – Re-think current algorithms in terms of the primitives

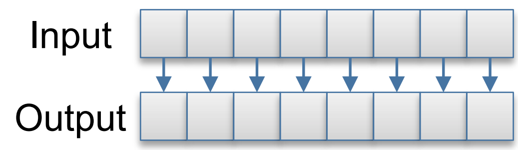


Data Parallel Primitives (DPP)

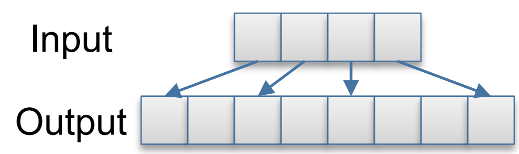
- What are they?
  - Provide a level of abstraction based on Blelloch's parallel primitive operators
  - Provides node level parallelism
- Big challenge
  - "re-thinking" algorithms to use DPP
  - Not "porting" algorithms to DPP
- Benefits
  - Portable performance
  - Future proof implementations
- What is a DPP
  - If it can be completed in O(logN) where N is the array size than it can be a DPP

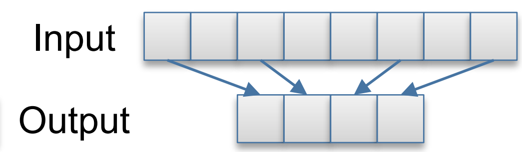
Data Parallel Operations

- Map
  - Parallel for each loop

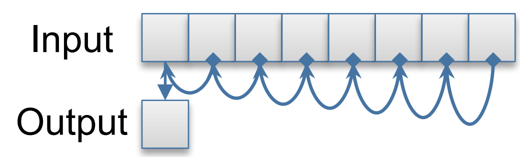


- Gather / Scatter
  - Index set array operations





- Scan
  - Index creation scheme
- Reduce
  - Counting / Narrowing results



Portable Performance – Abstraction Layer

- Previous work done in research group at UO
  - Ray Tracing
    - Promising results
    - Using VTK-m, EAVL, etc…
- Applying this technique to Monte Carlo Transport
  - Many possible avenues to consider
    - Thrust
      - supports data parallel operations
    - RAJA style
      - Supports simplifying key ideas with a template/MACRO definition

Monte Carlo Transport – ALPS_MC

- Models particle transport in a 1D binary stochastic medium
- Particles are created and then tracked through a series of events
- Tallies of multiple types are incremented
  - Single Value: Reflection, Transmission
  - Multi Value (per material): Absorption, Scatter
  - Many Value (per zone): Zonal Flux
- Legacy approach (history-based) did not lend itself to many-core
- Recent work takes a new approach (event-based) that is suitable for many-core systems

  (Investigation of Portable Event-Based Monte Carlo Transport Using the NVIDIA Thrust Library. in press.)

Event based algorithm - overview

- Determine a batch size
  - How many particles fit in GPU memory

- For a given batch
  - Generate all particles in batch
  - While any particles left to compute
    - For each event X
      - Get particles whose next event is X
      - Do event X and compute their next event
    - Delete killed particles

- 3 events tracked
  - Collision
  - Material interface crossing
  - Zonal boundary crossing

- Excluded zonal flux tally as future work to study its effect

AOS and SOA Particle Data Structure

- Particle class contains many variables
  - (3 ints, 1 Long, 6 doubles)
  - Real case scenarios contain even larger classes
- Not all variables used in each kernel
  - Reduce size of memory reads and writes
- Coalesced memory access with SOA
- Reduced memory usage in kernel

New Particle Removal Scheme

- Reorganizing particles is costly
  - More costly then all compute kernels combined
- Only call remove function when it makes an impactful change to array size
- If number to kill >= particles_remaining.size() / 2;
  - Decreases amount of time spent removing particles
  - Increase amount of time needed to establish compute kernels

Details of Implementation

- Explicitly managed GPU memory (cudaMalloc, etc.)
- Modified CUDA version first
  - Made new Thrust, RAJA methods from optimized CUDA method
- Changed particle data structure to allow SOA or AOS
- Kernels read/write strategy changed to ensure - read, compute, write pattern upheld
- New particle removal scheme

Results – 10 Million Particle Study

- Studies in CUDA to understand performance

(runtime in seconds)	SOA	AOS	SOA (kill/2)	AOS (kill/2)	SOA (sort)
Collision	0.77	0.89	0.93	1.03	0.92
Zone Boundary	0.62	0.79	0.75	0.93	0.74
Material Interface	0.70	1.11	0.92	1.33	0.91
Compute Total	2.09	2.80	2.59	3.28	2.57
Remove / Sort	3.95	2.31	0.36	0.42	1.08
Total Time	6.04	5.11	2.95	3.70	3.65

Results – 100 Million Particle Study

- Using one GPU device (½ K80)
  - Results From Paper:

(runtime in seconds)	AOS
Serial	508.74
Thrust	234.30
CUDA	48.39

  - Newest Results:

(runtime in seconds)	AOS	% slowdown	SOA	% slowdown
CUDA	38.68	-	31.43	-
Thrust	57.77	33%	33.84	8%
RAJA Like	42.10	8%	31.92	2%

Conclusion

- Spending time to make the SOA changes and directly managing CUDA memory paid off in performance for all versions
- Starting with CUDA, backing out an abstraction layer was simple
- Initial pass abstraction layer attempt suffered significant performance degradation
  - Lessons learned now can pay off down the line in future attempts at starting with an abstraction layer
- DPP portable performance approach promising for event based Monte Carlo transport

Acknowledgements

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Results – 80 Million Particles Study

- Using 1 GPU device (½ K80)

(runtime in seconds)	AOS	% slowdown	SOA	% slowdown
CUDA	1.00	-	0.79	-
Thrust	1.99	49%	1.38	43%
RAJA Like	1.17	15%	0.79	0%

- Using 4 GPU devices (2 K80s)

(runtime in seconds)	AOS	% slowdown	SOA	%slowdown
CUDA	0.27	-	0.23	-
Thrust	0.91	70%	0.78	71%
RAJA Like	0.32	16%	0.23	0%

Results – 100 Million Particle Study cont.

- Using 4 GPU devices (2 full K80s)

	AOS	SOA
CUDA	17.74 [s]	15.84 [s]
Thrust	18.34 [s]	11.37 [s]
RAJA Like	18.64 [s]	15.92 [s]

- Thrust SOA method scaling on multiple devices more effectively
- Only minor performance losses using RAJA over direct CUDA

Results – CPU Portability

- 100 Million Particle Study – Done on CPU
  - [SOA AOS]
  - Thrust: XXX.XX XXX.XX
  - RAJA like: XXX.XX XXX.XX
  - Thrust History: XXX.XX
  - OMP History: XXX.XX

- Comment on OMP results
- Comment on Portability of event versus history

[results not yet determined]